第15卷 第2,3期 广东有色金属学报 Vol. 15, No. 2,3
2005年9月 JOURNAL OF GUANGDONG NON-FERROUS METALS Sep 2005

Article ID: 1003-7837(2005)02,03-0164-04

Influence of inhomogeneity of grain-boundary region of nanocristalline materials on elastic properties*

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Abstract: Experimental data indicate that Young's modulus of materials decreases with the decreasing of the grain size. Obviously, the primary factor of this decrease is presence of grain-boundary region, which Young's modulus other than in the bulk of crystallites. There is a set of various expressions for calculation of Young's modulus of polycrystals, obtained under the assumption, that it is possible to consider a polycrystal as a composite consisting of a crystalline matrix and a intercrystalline layers (grain-boundary region). Calculations showed incorrectness of application of a majority of these expressions and a large error in the calculations for the nanocrystalline materials. By us, on the basis of the same assumptions, is also obtained analytical expression for calculating Young's modulus of materials with grain size more than 30 nm, which is more exact, than all others.

It is necessary to consider under the calculation of effective Young's modulus nanocrystalline materials with grain size of less than 30nm, that grain-boundary region itself is not uniform. It is reliably established, that the triple joints of grain boundaries have a structure and properties, different from the structure and the properties of grain boundaries, which these joints connect. For nanocrystalline materials the volume fraction of the triple joints in the grain-boundary region can reach 50% and even more. Therefore assumption was made, that the nanocrystalline materials should be represented as consisting of three phases (triple joints, grain boundary between the triple joints and crystallite). On the basis of this idea is obtained analytical expression for calculating of Young's modulus nanocrystalline materials. The analysis shows that Young's modulus calculated by this analytical expression coordinated with the theory and the experiment.

CLC number: TF77 **Document code**: A

The data on nanocrystalline materials Young's modulus measurement show it to have less value comparing with this of polycrystalline materials. Effective bulk Young's modulus decreases as grain size decreases. One of possible and, eventually, main factors for this decrease is the presence of grain-boundary phase where Young's modulus is different from one for grain itself. As it is shown in[1], the application of Reuss, Voigt and three-dimensional models for the calculation of nanocrystalline materials Young's modulus is incorrect. With the help of model proposed in [1], the analytical expression for the calculation of nanocrystalline materials effective Young's modulus was received. It is the combination of Young's modulus for grain-boundary phase and one for crystalline matrix and also depends on the volume fraction of grain-boundary phase in the crystal bulk. One should notice that the analytical expression for the calculation of material

Received date: 2005-08-29

* **Foundation item**: supported by RFBD under grant No 05-03-33088

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Young's modulus received in[1] has the accuracy not higher than 4% for the materials with grain size less than 30 nm. That accuracy decreases as grain size decreases. This takes place because grain-boundary phase isn't homogenious.

It is established for sure that grain-boundaries triple junctions have the structure and properties different from those of grain-boundaries themselves [2]. In nanocrystalline materials the volume fraction of triple junctions may reach 50% and above[3]. Therefore, in the procedure of effective Young's modulus calculation the nanomaterial with grain size above 30 nm can be considered as consisting of two phases (grain-boundary phase and crystallite) with the accuracy 4%, but, at the same time, we should consider the nanomaterial with grain size less 30 nm as consisting of three phases (triple junctions, grain-boundaries between triple junctions, and crystallite).

In the given article the analitical expression obtained for different nanomaterials effective Young's modulus depending of Young's moduluses for crystallite, triple junctions, and grain-boundaries between triple junctions and depending of grain size.

Let us consider a ball-shape sample with volume V and grain size d. Let us suppose that the aggregate volume of triple junctions in the sample is V_S, the aggregate volume of grain boundaries between triple junctions is V_B, and the volume of intergrain substance is V_0. Then $V=V_S+V_B+V_0$.

The volume fraction of grain-boundary phase consisting of grain boundaries triple junctions and grain boundaries between triple junctions, α can be estimated by formula [4]:

$$\alpha=1-\left(\frac{d-\delta}{d}\right)^3, \tag{1}$$

where $\delta = 1$ nm (the thickness of grain-boundary phase).

The volume fraction of grain boundaries triple junctions, α_S can be calculated by formula[4]:

$$\alpha_S=\left(3-2\frac{\delta}{d}\right)\left(\frac{\delta}{d}\right). \tag{2}$$

Let us suppose that uniform compression pressure σ, lower than the elastic limit, is applied to the sample. Then Hooke's law is applicable:

$$\sigma=E\cdot\Delta l/l \tag{3}$$

where E is Young's modulus averaged over the sample volume, l is the initial linear size of the sample (ball's diameter), Δl is the change of sample linear size due to uniform compression.

The initial linear size of the sample along the OX axis put through the ball's center is the sum of aggregate linear size of grain-boundary phase that cross the OX axis and aggregate linear size of intergrain phase along the OX axis. Therefore:

$$l=l_S+l_B+l_0, \tag{4}$$

where l_S, l_B, l_0 are aggregate linear sizes of grain boundaries triple junctions, grain boundaries between triple junctions, and intergrain phase, respectively.

The total sample compression is a sum of grain-boundary phase compression and intergrain phase compression. Therefore:

$$\Delta l=\Delta l_S+\Delta l_B+\Delta l_0, \tag{5}$$

where Δl_S, Δl_B, Δl_0 are the changes of aggregate linear sizes of grain boundaries triple junctions, grain boundaries between triple junctions, and intergrain phase, respectively.

Hooke's law is valid for each of those three phases separately, therefore:

$$\sigma=E_S\frac{\Delta l_S}{l_S}, \tag{6}$$

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$$\sigma=E_B\frac{\Delta l_B}{l_B}, \tag{7}$$

$$\sigma=E_0\frac{\Delta l_0}{l_0}, \tag{8}$$

where E_S, E_B and E_0 are Young's moduluses for grain boundaries triple junctions, grain boundaries between triple junctions, and crystallite, respectively.

It follows from (3-8) that:

$$\frac{l_0+l_S+l_B}{E}=\frac{l_0}{E_0}+\frac{l_S}{E_S}+\frac{l_B}{E_B}. \tag{9}$$

In the framework of the adopted model, the ratio of different phases volumes to sample volume is equal to the cubic relation of linear sizes along OX axis for those phases to the sample size. Therefore:

$$\frac{l_0}{l_0+l_S+l_B}=\frac{l_0 l}{l_0 l+l_S l+l_B l}=\frac{\sqrt[3]{V_0/V}}{\sqrt[3]{V_0/V}+\sqrt[3]{V_S/V}+\sqrt[3]{V_B/V}}=\frac{\sqrt[3]{1-\alpha}}{\sqrt[3]{1-\alpha}+\sqrt[3]{\alpha_S}+\sqrt[3]{\alpha-\alpha_S}}, \tag{10}$$

$$\frac{l_S}{l_0+l_S+l_B}=\frac{\sqrt[3]{\alpha_S}}{\sqrt[3]{1-\alpha}+\sqrt[3]{\alpha_S}+\sqrt[3]{\alpha-\alpha_S}}, \tag{11}$$

$$\frac{l_B}{l_0+l_S+l_B}=\frac{\sqrt[3]{\alpha-\alpha_S}}{\sqrt[3]{1-\alpha}+\sqrt[3]{\alpha_S}+\sqrt[3]{\alpha-\alpha_S}}. \tag{12}$$

Taking into account equations (10), (11), and (12), one can find from equation (9):

$$\frac{\sqrt[3]{1-\alpha}+\sqrt[3]{\alpha_S}+\sqrt[3]{\alpha-\alpha_S}}{E}=\frac{\sqrt[3]{1-\alpha}}{E_0}+\frac{\sqrt[3]{\alpha_S}}{E_S}+\frac{\sqrt[3]{\alpha-\alpha_S}}{E_B}. \tag{13}$$

Let us find E_S and E_B by the help of equation (13), using the experimental data for gold[5] given in Table 1. Taking E and E_0 for different grain sizes and for one and the same temperature, we get the system of two equations with two unknown quantities E_S and E_B.

The results of E_S and E_B calculation by formula (13) for gold are given in Table 2. One can see from this table that E_S and E_B values are very different from each other. This gives us a hint that the most "weak" objects in the sample are the grain boundaries triple junctions and possibly this is why the crack nucleation in metal usually takes place in grain-boundary region and in junctions.

Table 1

Material	d/nm	T/K	E/GPa	E_0/GPa
Gold	26	80	77±1	84 0.5
Gold	60	80	79±1	84 0.5
Gold	26	200	73.5±1	80 0.5
Gold	60	200	75.5±1	80 0.5

Table 2

T/K	E_S/GPa	E_S/E_0	E_B/GPa	E_B/E_0
80	50.9	0.61	77.6	0.92
200	46.5	0.58	76.2	0.95

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